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Results from an International Simulation Study on Coupled Thermal, Hydrological, and Mechanical (THM) Processes near Geological Nuclear Waste Repositories

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Abstract – *As part of the ongoing international code comparison project DECOVALEX, four research teams used five different models to simulate coupled thermal, hydrological, and mechanical (THM) processes near underground waste emplacement drifts. The simulations were conducted for two generic repository types with open or back-filled repository drifts under higher and lower post-closure temperature, respectively. In the completed first model inception phase of the project, a good agreement was achieved between the research teams in calculating THM responses for both repository types, although some disagreement in hydrological responses are currently being resolved. Good agreement in the basic thermal-mechanical responses was achieved for both repository types, even with some teams using relatively simplified thermal-elastic heat-conduction models that neglect complex near-field thermal-hydrological processes. The good agreement between the complex and simplified (and well-known) process models indicates that the basic thermal-mechanical responses can be predicted with a relatively high confidence level. The research teams have now moved on to the second phase of the project, the analysis of THM-induced permanent (irreversible) changes and the impact of those changes on the fluid flow field near an emplacement drift.*

I. INTRODUCTION

This paper presents results from an international multiple-team simulation study on thermal, hydrological, and mechanical (THM) interactions around underground nuclear waste emplacement drifts. The study is part of the ongoing DECOVALEX-THMC project described in detail by Birkholzer et al. [1]. The general goal of the project is to encourage multidisciplinary, interactive, and cooperative research on modeling coupled processes in geologic formations in support of the performance assessment for underground storage of radioactive waste. The main processes studied in the case of THM are (1) heating of the rock mass with associated thermally induced stresses, (2) thermal-mechanically induced changes in hydrological rock properties, and (3) changes in the fluid flow distribution around waste emplacement drifts. Two generic repository types with horizontal emplacement tunnels are considered within the project:

Type A) A high temperature (above boiling) repository in a deep unsaturated volcanic rock formation with emplacement in open gas-filled tunnels, similar to the Yucca Mountain Project concept.

Type B) A low temperature (below boiling) repository in a deep saturated crystalline rock formation with emplacement in back-filled tunnels, a concept considered in many European countries and Japan.

The initial rock properties for the two repository types are derived from measurements and previous DECOVALEX analyses of two major *in situ* experiments, representing data and processes occurring at the two repository types. The first one, representing Repository Type A, is the Yucca Mountain Drift Scale Test, conducted at Yucca Mountain, Nevada [2]. The second one, representing Repository Type B, is the FEBEX *in situ* experiment, conducted at the Grimsel Test Site, Switzerland [3]. Previous THM simulations of these two major field experiments have already demonstrated that the short-term (occurring over several years) coupled THM processes are well understood. In the present study, however, the models are used to predict coupled THM processes over tens of thousands of years.

Four international teams from China, Germany, Japan, and USA are participating in this task (see Table

1). Altogether, five different numerical codes for coupled THM analysis are applied. DOE uses two alternative codes, TOUGH-FLAC (which is widely used within the Yucca Mountain Project) and ROCMAS. JAEA uses a code called THAMES, BGR uses the GeoSys/Rockflow family of codes, and CAS uses FRT-THM, which utilizes the general-purpose FEMLAB multi-physics software (see Table 1 for a short description of each numerical simulator).

II. SIMULATION TASKS

Research teams participating in the research task are asked to conduct predictive analysis of the long-term coupled THM processes for the two repository types. The simulations are conducted on two-dimensional drift-scale models containing one horizontal emplacement tunnel, which for each repository type has different dimensions and thermal load (Figure 1). Participating research teams model the THM processes in the fractured rock close to the representative emplacement tunnel as a function of time, predict the changes in hydrological properties, and evaluate the impact on near-field flow processes. The simulations to be conducted include three phases:

Phase 1. Model inception

Phase 2. Preliminary model prediction and sensitivity analysis

Phase 3. Final model prediction with uncertainty range

The purpose of the model inception phase (Phase 1) is for the research teams to familiarize themselves with the problem by performing one simulation in which all the properties are explicitly provided (Table 2). Thus, in this phase no data or model uncertainties are considered, and changes in hydrological properties are neglected. The results of the research teams are compared even at this stage to assure that they are starting the problem on a common basis before further complexities are added in Phases 2 and 3. In Phase 2, the research teams are to develop their model and input material properties from available site data, with the ultimate goal of predicting mechanically induced permanent changes. In Phase 3, the research teams are asked to make their final prediction, along with an evaluation of the uncertainties in their prediction.

III. THM SIMULATION RESULTS

Currently all teams have completed the necessary model development and have provided results for Phase 1 (model inception). Thus, this paper presents results of Phase 1.

III.A Thermal-Mechanical Results

Figure 2 schematically illustrates simulation results of coupled thermal-mechanical responses. The main thermal-mechanical responses are a result of regional thermal stressing induced by regional temperature changes in the rock mass (Figure 2a). A substantial increase in thermal stress in the horizontal direction occurs as a result of lateral confinement of the rock mass, whereas vertical stress is much less affected as the free moving ground surface allows for vertical expansion. The regional thermal stressing is amplified at the drift wall by stress redistribution causing highly compressive stress at the top and bottom of the drift and strong stress relief at the right and left side (Figure 2b).

Figure 3 shows comparisons of temperature and stress-evolution calculated using the five different models. The figure shows a generally good agreement for temperature and stress evolution, especially in the case of Repository Type A (Figure 3a). The more significant deviations in temperature evolution that can be seen for Point V1 for Repository Type B (Figure 3b) can be explained by differences in the evolution of saturation-dependent thermal conductivity in the backfill. The observed disagreement in thermal stress by one model (dashed line in Figure 3c and d), is a result of a misconception of the initial stress and excavation modeling. One purpose of Phase 1 (model inception) is to eliminate such misconceptions and eliminate differences in the basic underlying thermal-mechanical calculations before moving on to Phase 2.

The main difference between thermal-mechanical responses in Repository Type A and B, is related to the evolution of the heat-power and the thermal stress magnitude in comparison with the initial stress field. In Type A, the thermally induced stresses are a little lower, but at the same time the initial stresses in that case are much smaller. Furthermore, in Type A, the thermal stresses causesthe principal *in situ* stress field to rotate, from the initial maximum principal stress being vertical to becoming horizontal at the time of peak thermal stress. In Type B, on the other hand, the *in situ* stresses are initially already relatively high, with the maximum principal stress being horizontal. In this case, the thermal stressing provides an additional increase in the horizontal stress, without rotation of the *in situ* principal stress field.

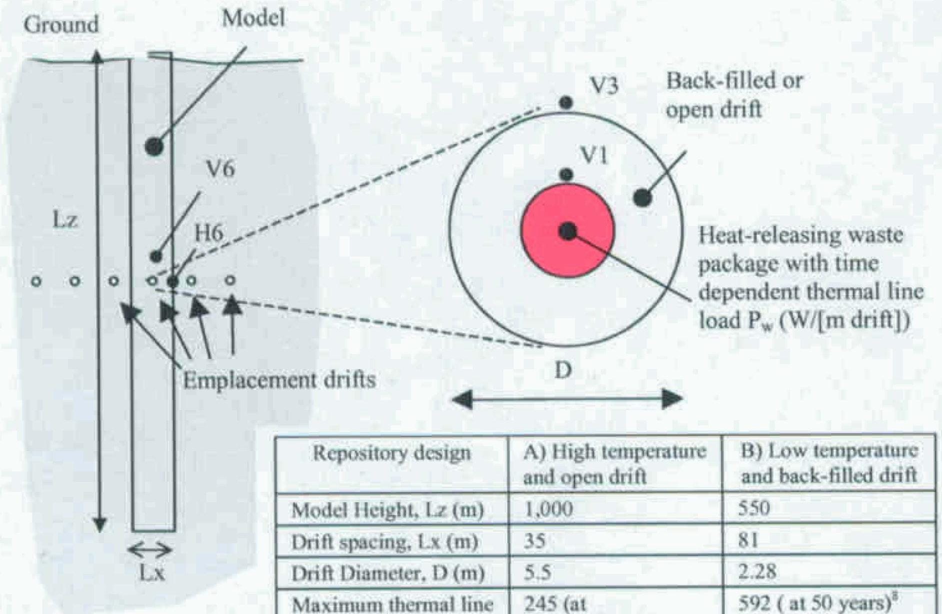
TABLE 1: Research teams and simulators applied in this study

Research Team	Numerical Simulator	Brief Description of Numerical Simulator
DOE U.S. Department of Energy's Research Team: Lawrence Berkeley National Laboratory (LBNL)	**TOUGH-FLAC**	TOUGH-FLAC is a simulator for analysis of coupled THM processes under multiphase fluid flow conditions developed at the LBNL in the last few years. The simulator is based on linking of the existing computer codes TOUGH2 and FLAC3D. It has been extensively used for analysis of coupled THM processes within the Yucca Mountain Project.
	ROCMAS	ROCMAS is a finite element program for analysis of coupled THM processes in porous and fractured rock developed at LBNL since the late 1980s. In the late 1990s, this code was extended to unsaturated media with single-phase liquid flow and vapor diffusion in a static gas phase. The code has been extensively applied in earlier phases of the DECOVALEX project for THM analysis in bentonite-rock systems.
BGR Bundesanstalt für Geowissenschaften und Rohstoffe's Research Team: University of Tübingen	**GeoSys/ Rockflow**	GeoSys/Rockflow is based on object-oriented programming and is developed at the University of Tübingen in the last few years. It was first applied in previous DECOVALEX phases for analysis of thermal-hydrological and thermal-mechanical processes and has recently been extended to THM analysis. For the present study, an unsaturated single-phase liquid flow and vapor diffusion is considered.
CAS Chinese Academy of Sciences' Research Team	**FRT-THM**	The FRT-THM (Fluid-Rock Transport simulator) being developed by the CAS is based on MATLAB and C language codes, in which FEMLAB is used as partial differential equation solver. The approach being developed for the present study features an unsaturated single-phase fluid flow and vapor diffusion model approach.
JAEA Japan Atomic Energy Agency's Research Team, including Hazama Cooperation	**THAMES**	THAMES is a finite element program for analysis of coupled THM processes in porous and fractured rock developed at the Kyoto University since the late 1980s. The code has been extended to unsaturated media with single-phase liquid flow and vapor diffusion in a static gas phase. The THAMES code has been extensively applied in earlier phases of the DECOVALEX project for THM analysis in bentonite-rock systems.

TABLE 2. Some basic rock properties defined for Phase 1 (Model Inception).

Parameter	Repository Type A (Welded Tuff)[1)]	Repository Type B (Granitic)
Bulk Density, [kg/m^3]	2370	2700
Matrix Porosity [-]	0.13	0.01
Young's Modulus, [GPa]	15	35
Poissons ratio, [-]	0.21	0.3
Specific heat, [J/kg·°C]	985	900
Thermal conductivity, [W/m·°C]	2.29 (wet)	3.0
Thermal expan, coefficient [1/°C]	1.0×10^{-5}	$1\cdot10^{-5}$
Permeability, [m^2]	3.3×10^{-13} (fracture continuum)	1×10^{-17} (bulk)

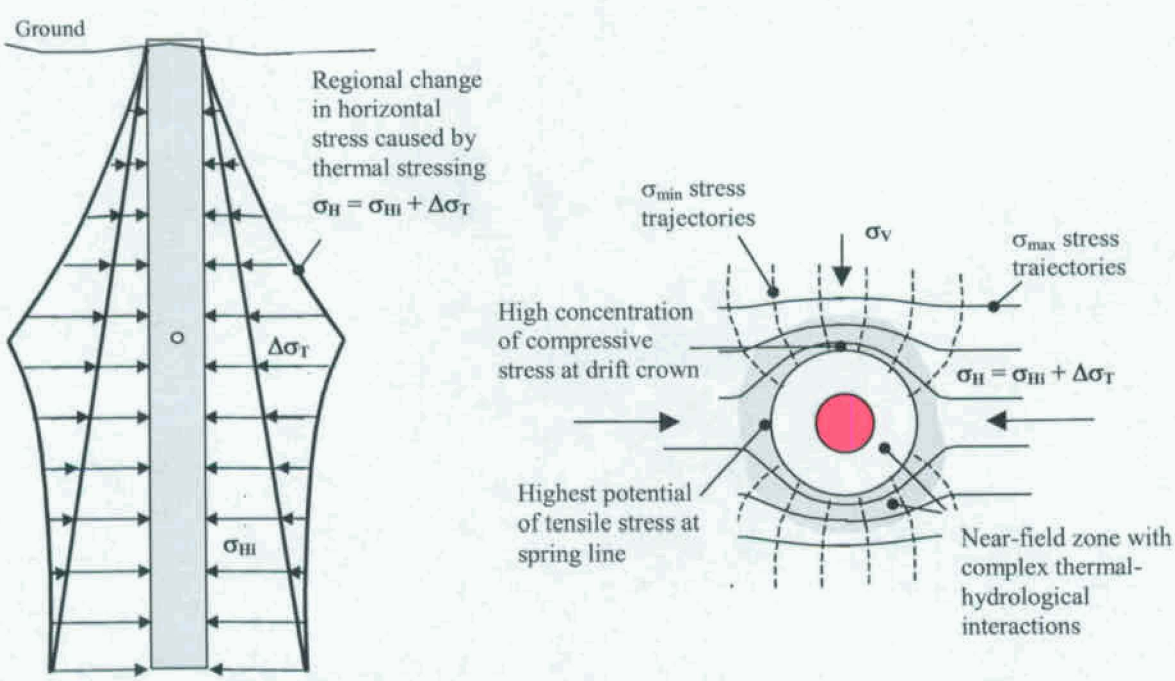
[1] The complete data set for welded tuff includes multiphase (e.g., retention and relative permeability data for gas and liquid) fluid flow properties for matrix and fracture continua.



Repository design	A) High temperature and open drift	B) Low temperature and back-filled drift
Model Height, Lz (m)	1,000	550
Drift spacing, Lx (m)	35	81
Drift Diameter, D (m)	5.5	2.28
Maximum thermal line load, Pw (W/m)	245 (at emplacement)	592 (at 50 years)*

* Heat load is reduced by drift ventilation until 50 years

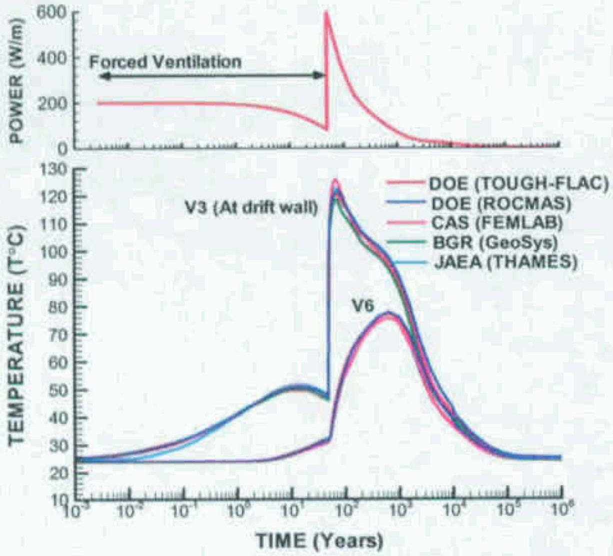
Figure 1. Two-dimensional model geometry for analysis of the two repository types (A and B) and location of some output points.



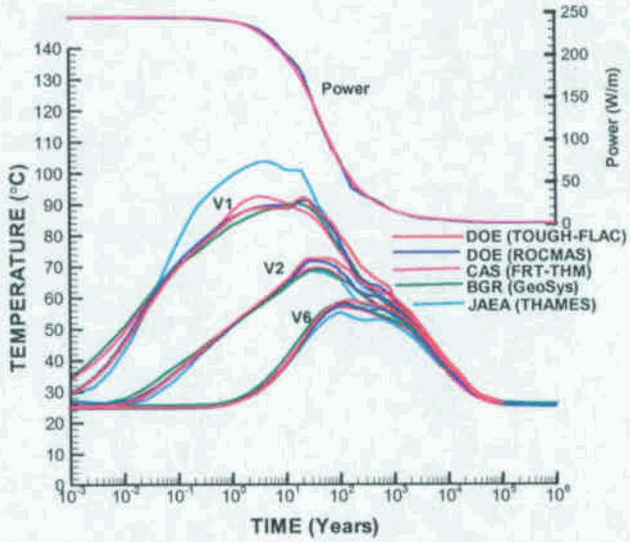
(a) Regional Changes in Horizontal Stress

(b) Near-field stresses as a result of regional stress changes

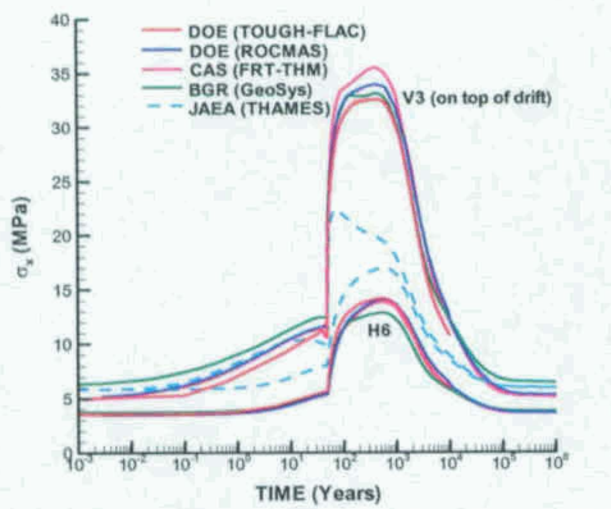
Figure 2. Schematic of main thermal-mechanical responses common for both Repository Type A and B.



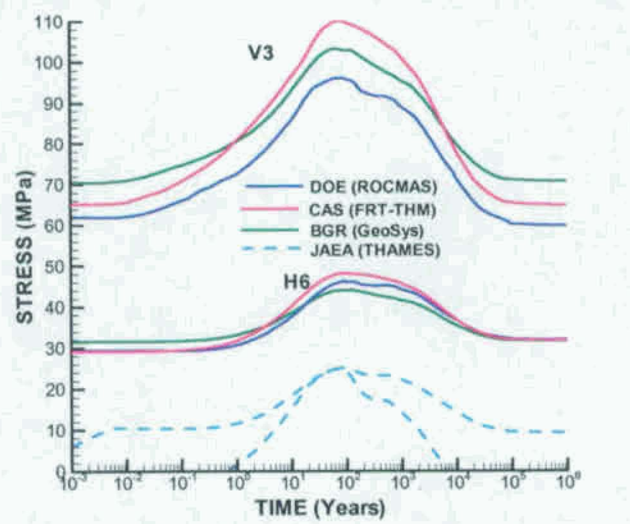
(a) Power and temperature evolution for Repository Type A



(b) Power and temperature evolution for Repository Type B

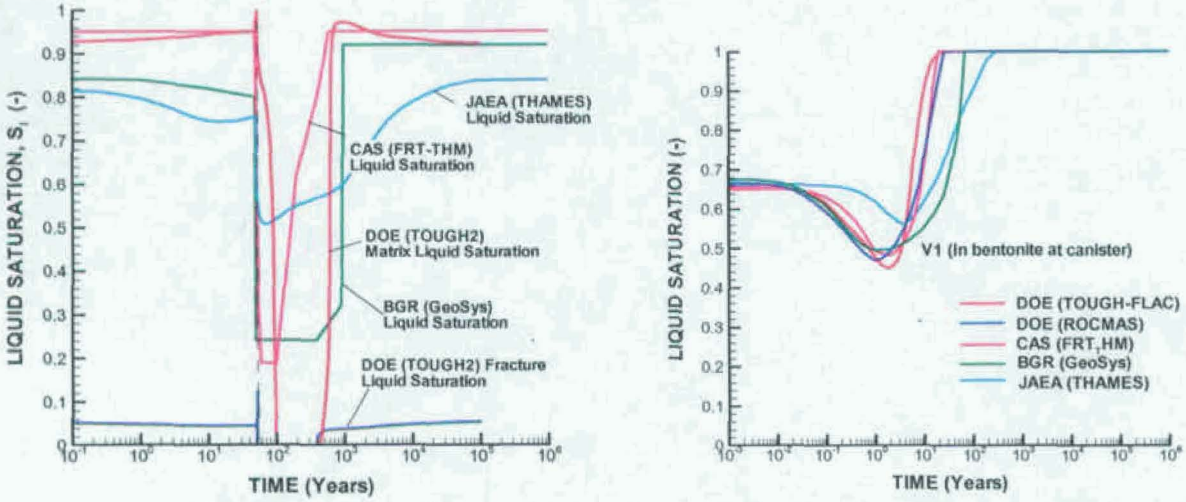


(c) Evolution of Horizontal stress for Repository Type A



(d) Evolution of Horizontal stress for Repository Type B

Figure 3. Evolution of thermal-mechanical responses for Repository Type A (high temperature open drift) and B (low-temperature back-filled drift) repository. Approximate locations of Points V1, V3, V6, and H6 are given in Figure 1 and explanations of acronyms DOE, CAS, BGR, and JAEA are given in Table 1.



(a) Evolution in point V3 for Repository Type A

(b) Evolution in Point V1 for Repository Type B

Figure 4. Evolution liquid saturation for Repository Type A (high temperature open drift) and B (low temperature back-filled drift) repository.

III.B Thermal-Hydrological Results

Thermal-hydrological simulation results studied and compared in Phase 1 include evolution of fluid pressure, saturation, and vertical flux.

Complex thermal-hydrological interactions occur in the near-field for both Repository Type A and B. In the case of Repository Type A, high temperatures cause boiling and complex heat-pipe effects, which result in drying of the rock near the drift wall. A dryout zone is created, which extends as much as a few meters from the drift wall into the surrounding rock mass. The simulation results indicates that such a dryout zone exists as long as the rock temperature near the drift exceeds the boiling points, which it does for a time period between 50 to about 1,000 years. In the case of Repository Type B, thermal-hydrological interactions are most prominent within the bentonite buffer. The bentonite buffer is installed and conditioned to an initial saturation of about 65%. During the initial few years of heating, a relatively steep thermal gradient causes evaporation of liquid water near the waste canister, with migration of vapor along the thermal gradient towards cooler regions of the buffer, where it condenses as liquid water. However, this initial drying is later overcome by seepage of liquid water from the fully saturated drift wall into the partially saturated buffer, and the buffer becomes fully saturated in about 10 to 50 years.

Figure 4 shows the comparison of the evolution of liquid saturation at two selected monitoring points, Point V3 10 cm into the drift wall in Repository Type A and Point V1 at the canister-buffer interface in Repository Type B (see Figure 1 for locations of V1 and V3). Whereas the agreement between different models for Repository Type B is quite satisfactory, the results for Repository Type A are more complex and show more significant deviations between the different teams. However, the comparison for Repository Type A is complicated by the fact that the results of single continuum models (BGR, JAEA, CAS) are compared to those of a more rigorous dual-continuum model (DOE, TOUGH-FLAC). In general, Figure 3a shows that the total dryout time till rewetting calculated by CAS (FRT-THM), DOE (TOUGH-FLAC) and BGR (GeoSys) models is similar, while the time evolution of saturation is somewhat different. The JAEA (THAMES) results indicate limitations in solving the above-boiling thermal-hydrological effects using the simplified single continuum approach. Better agreement is expected in future project phases, when more rigorous models (not just single continuum) will be used by all teams to simulate flow in fractures and matrix rock.

IV. EVALUATION OF MODEL APPROACHES

Results of the model inception phase show that good agreement was achieved in calculating THM responses for both repository types by various model approaches, thus demonstrating how different models and approaches can be adapted to both back-filled and open-drift systems. All models listed in Table 1 properly simulate the basic thermal-mechanical responses, including temperature and thermal stress evolution. All models are also capable of simulating coupled THM behavior under single-phase flow conditions in Repository Type B for the assumed simplified bentonite mechanical properties and equivalent continuum flow conditions. At the moment, only the TOUGH-FLAC code and its setup for full multiphase dual-continuum fluid flow and heat transport can properly simulate fluid flow for Repository Type A. However, with application of a dual-continuum approach or similar approaches that correctly accounts for fracture-matrix interactions, the results of other models could be much improved with regard to fluid flow, and hence the remaining deviations in the evolution of saturation near the drift wall can be resolved.

Despite some differences in the evolution of near-field thermal-hydrological processes, the agreement in predicted thermal-mechanical responses in the rock mass is good (see Figure 5). The near-field thermal-hydrological processes only affect the temperature evolution in the bentonite buffer and close to the drift wall, whereas these have a negligible effect on the regional temperature field. As a result, predictions of thermal-mechanical changes in the rock mass can be made with relatively simple models, neglecting detailed simulations the complex near-field thermal-hydrological processes. In fact, the regional temperature field could be well predicted with a pure conduction model controlled by the thermal conductivity and specific heat of the rock. Thus, if the purpose were only to predict thermal-mechanical responses, a relatively simple thermo-elastic, heat-conduction model would be sufficient. However, to accurately predict the impact of thermal-mechanical responses on permeability and the flow field, a proper fluid flow model, which includes fracture-matrix interactions, is necessary.

V. CONCLUSIONS AND DISCUSSION

In this paper, we present the progress of an international multiple-team study of coupled thermal, hydrological, and mechanical (THM) interactions associated with open and back-filled repository-drift designs in volcanic and crystalline rocks. A good agreement was achieved in calculated THM responses for both repository types, although deviations related to multiphase fluid flow and matrix-fracture interactions should be resolved. The results of the model inception phase demonstrate how different models and approaches can be adapted to both the systems of back-filled and open drifts. The study shows that predictions of thermal-mechanical changes in the rock mass can be made with relatively simple models, neglecting detailed simulations of some of the complex near-field thermal-hydrological processes. This finding implies that the basic thermal-mechanical stresses can be predicted with a relatively high confidence level. We conclude that the main purpose of Phase 1 has been achieved—to make sure that the teams accurately calculate basic thermal stress evolution, which is the driving force behind permanent changes in hydrological properties. The research teams will presently start with Phase 2, which is the preliminary model prediction and sensitivity analysis of permanent (irreversible) changes, and the impact of those changes on the fluid flow field around the emplacement drift. Those calculations will require a fully coupled THM analysis with accurate modeling of the fluid flow field, including fracture-matrix interactions.

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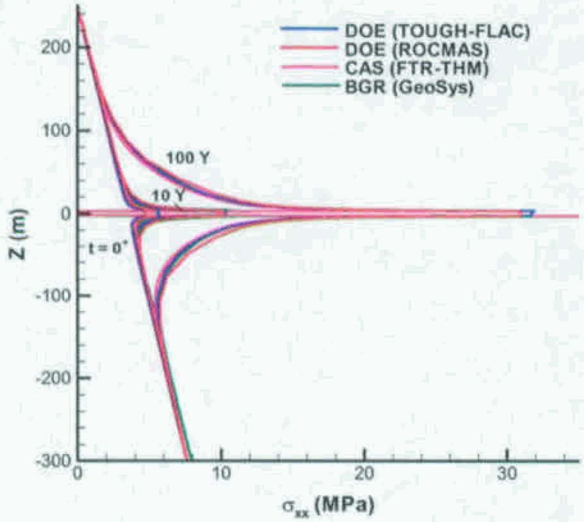
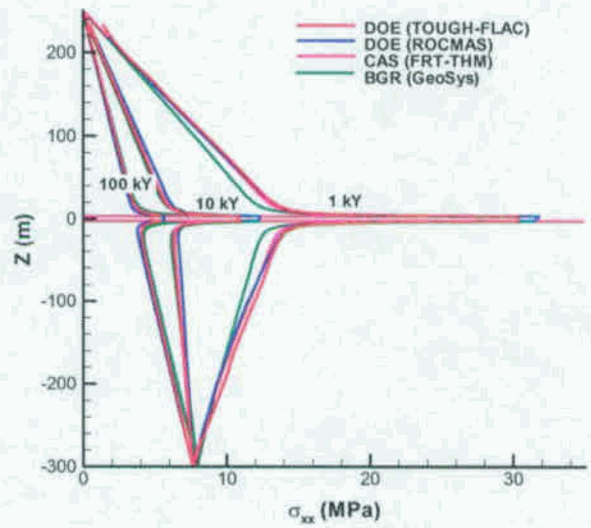
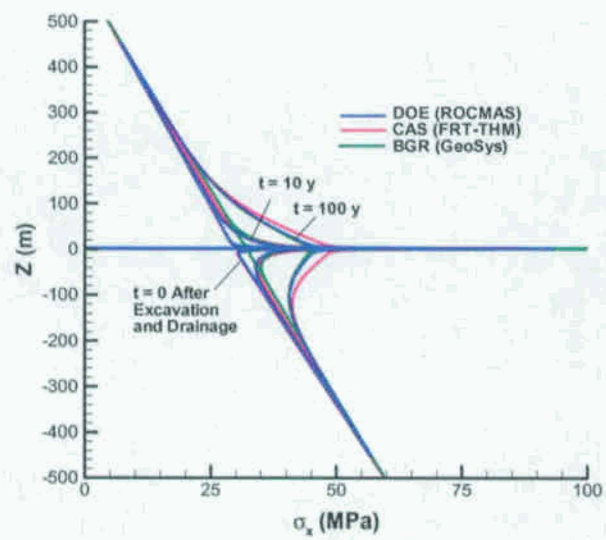


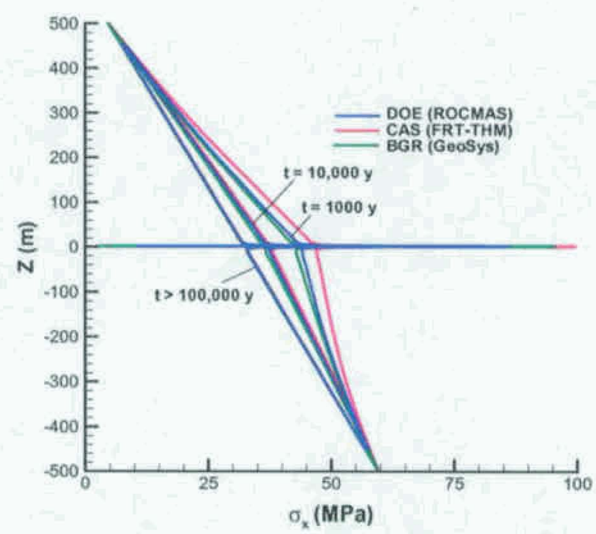
(a) Repository Type A (0 to 100 years)



(b) Repository Type A (0 to 100 years)



(a) Repository Type B (0 to 100 years)



(b) Repository Type B (0 to 100 years)

Figure 5. Comparison of simulation results for prediction of how regional horizontal stress evolves in Repository Type A (a and b) and Repository Type B (c and d).